UNIVERSITY OF CAMBRIDGE

Pseudizing the Hamiltonian

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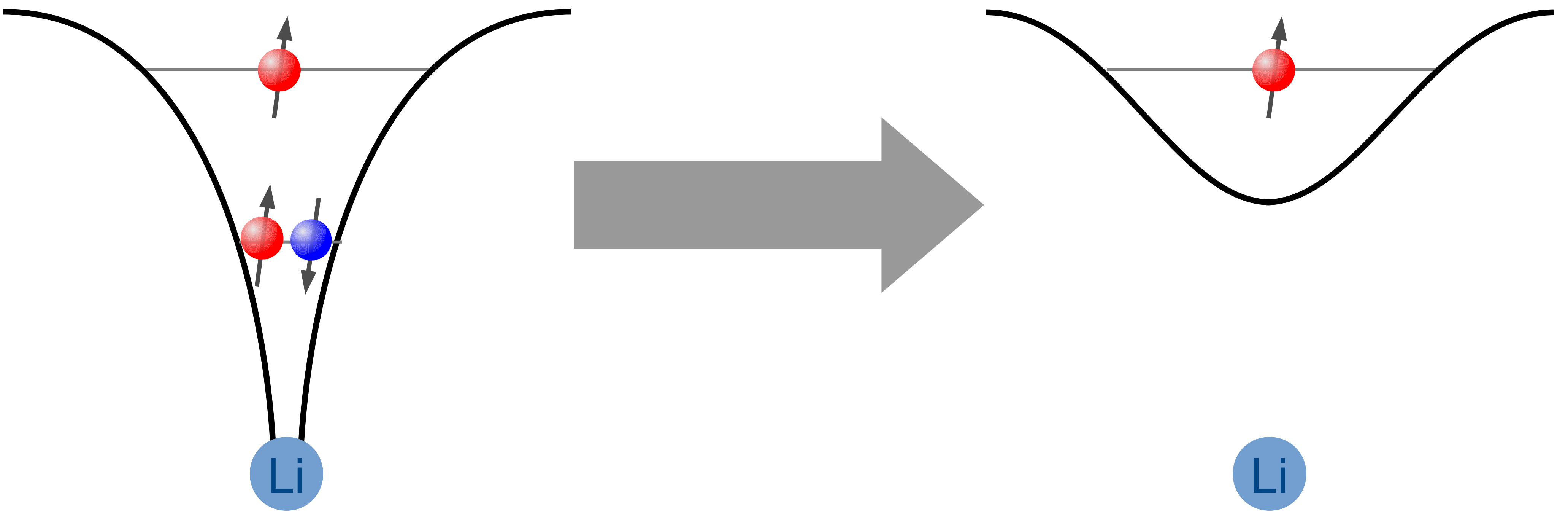
Hamiltonian

$$H = KE + V_{\text{e-i}} + V_{\text{e-e}}$$

$$E = \frac{\int \bar{\psi} H \psi \, \mathrm{d}\boldsymbol{r}}{\int \bar{\psi} \psi \, \mathrm{d}\boldsymbol{r}}$$

Electron-ion pseudopotential

$$H = KE + V_{\text{e-i}} + V_{\text{e-e}}$$

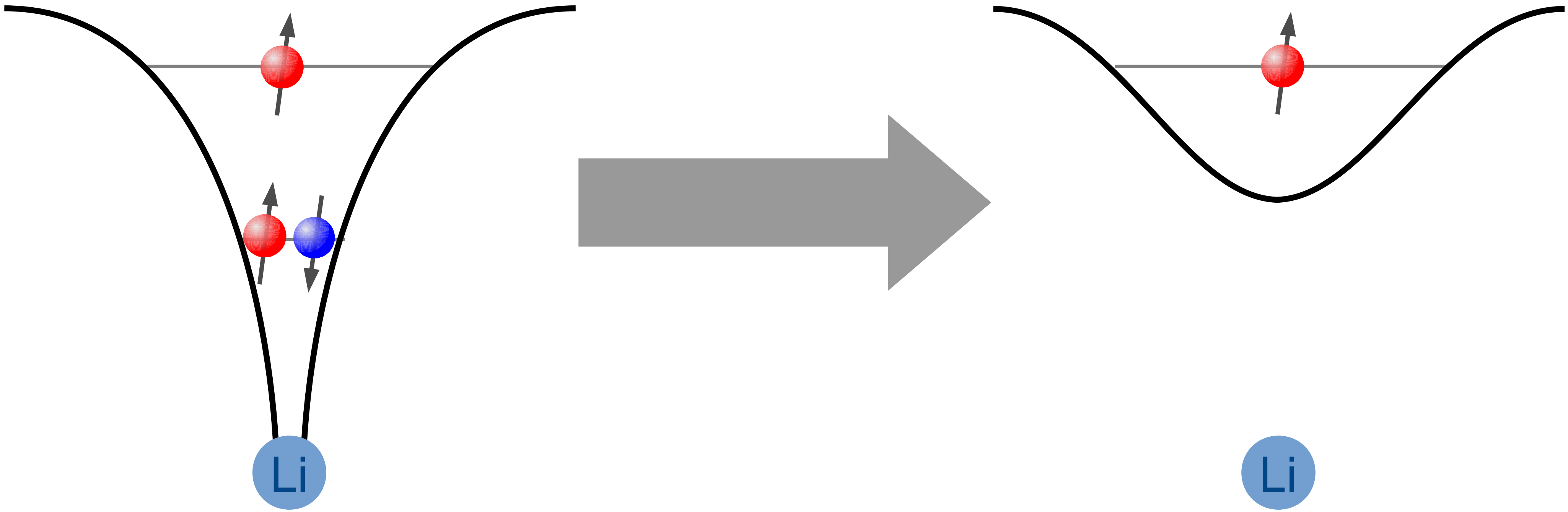


Electron-ion pseudopotential

$$H = KE + V_{\text{e-i}} + V_{\text{e-e}}$$

Fewer electrons

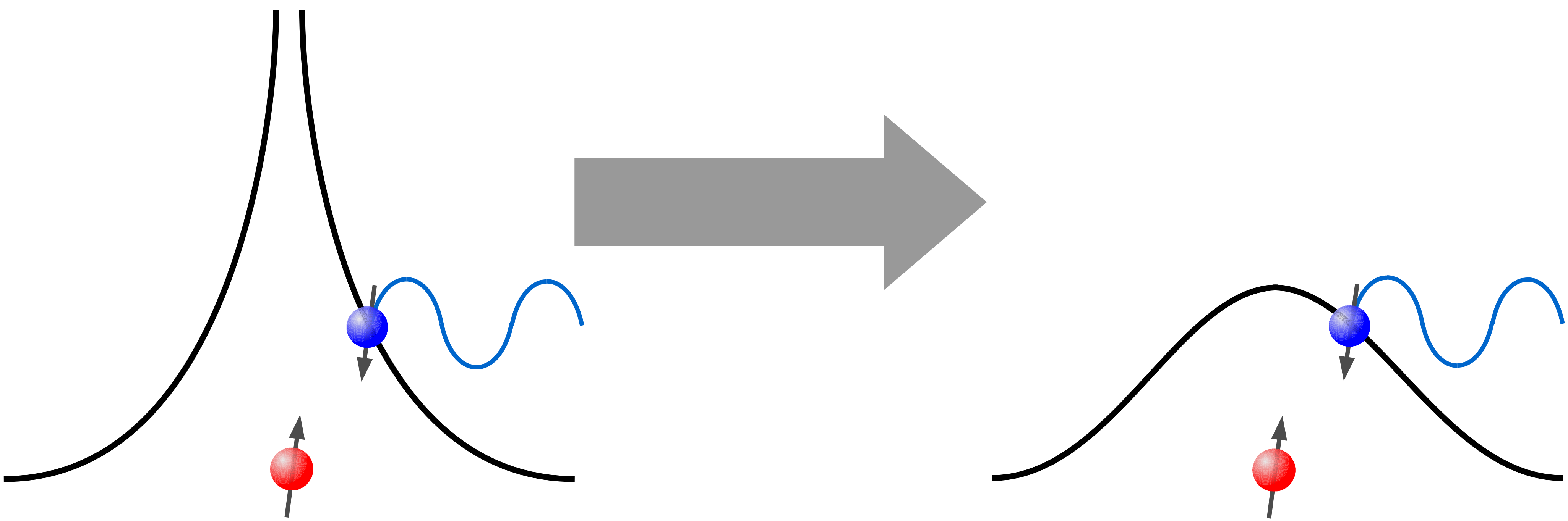
Smooth background



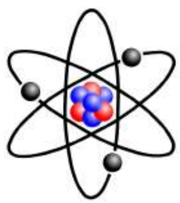
Electron-electron pseudopotential

$$H = KE + V_{e\text{-}i} + V_{e\text{-}e}$$

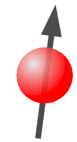
Smooth potential

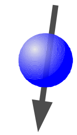


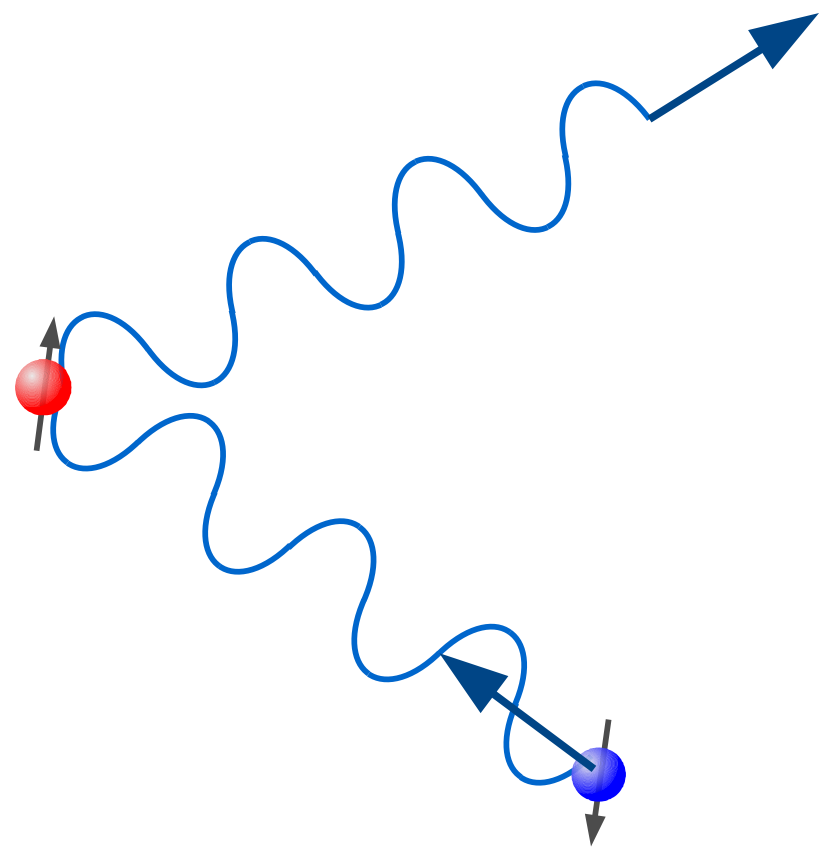
Scattering in ultracold atom gases



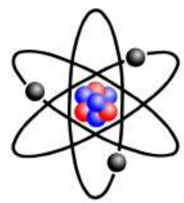
^{6}Li atom

$|F=1/2, m_F=1/2\rangle$ →  Up spin

$|F=1/2, m_F=-1/2\rangle$ →  Down spin



Scattering in ultracold atom gases



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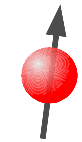
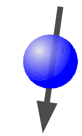
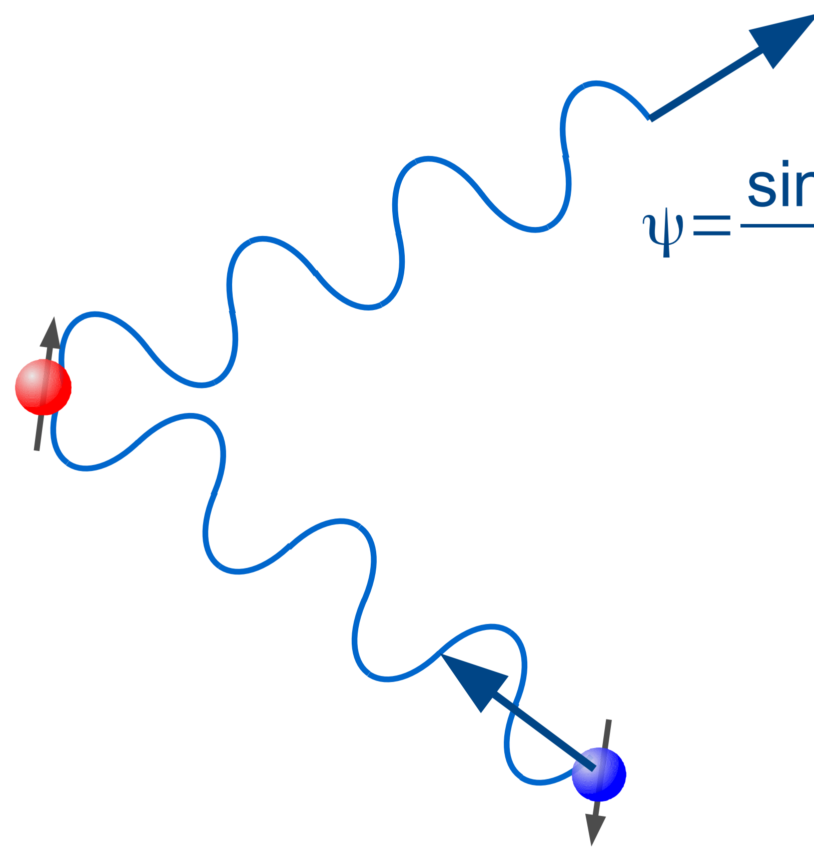
$|F=1/2, m_F=1/2\rangle$ →  Up spin

$|F=1/2, m_F=-1/2\rangle$ →  Down spin



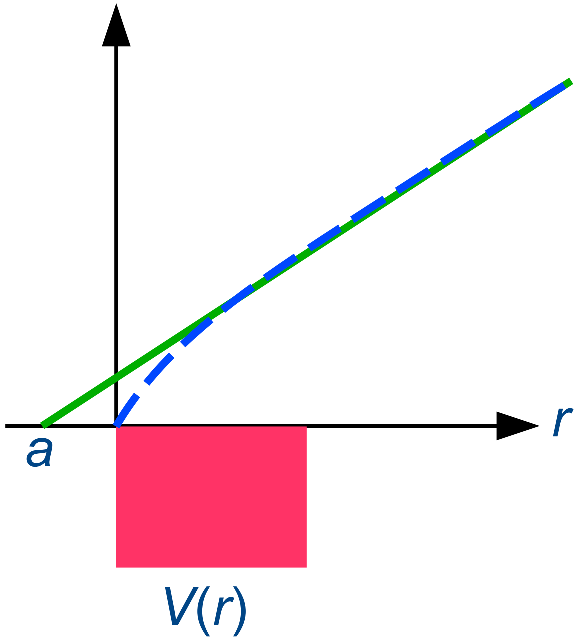
$$V(r)=4\pi a\delta(r)\frac{d}{dr}r$$

$$\psi=\frac{\sin(kr+\delta)}{kr}$$

Scattering potentials

Underlying attractive

Effective attractive



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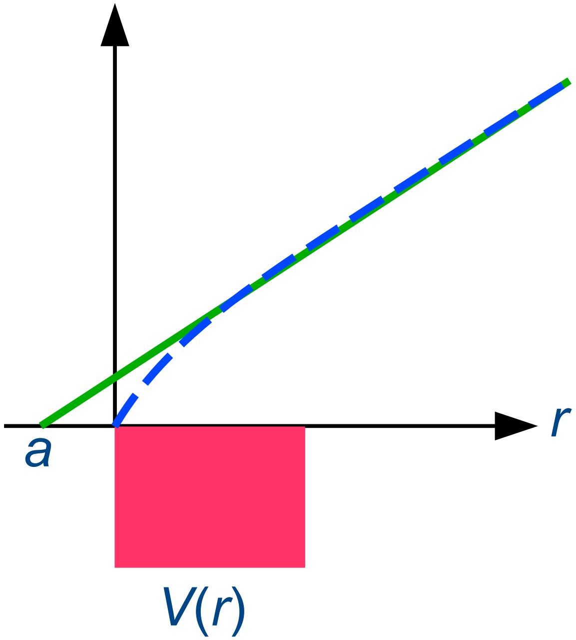
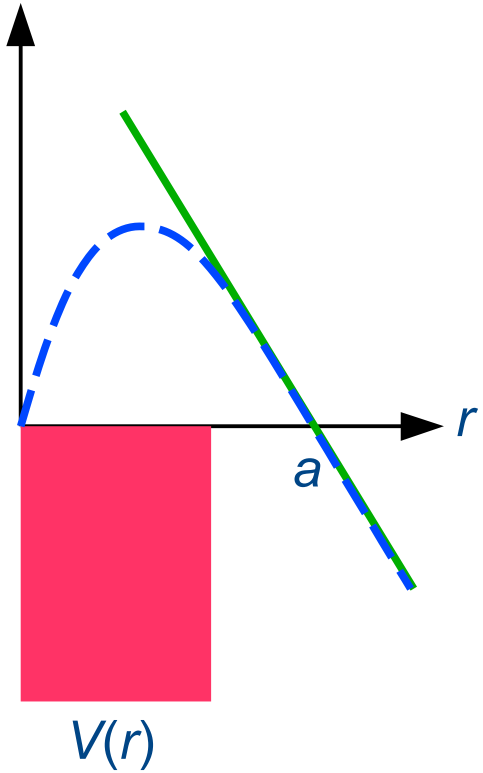


Underlying attractive

Effective repulsive



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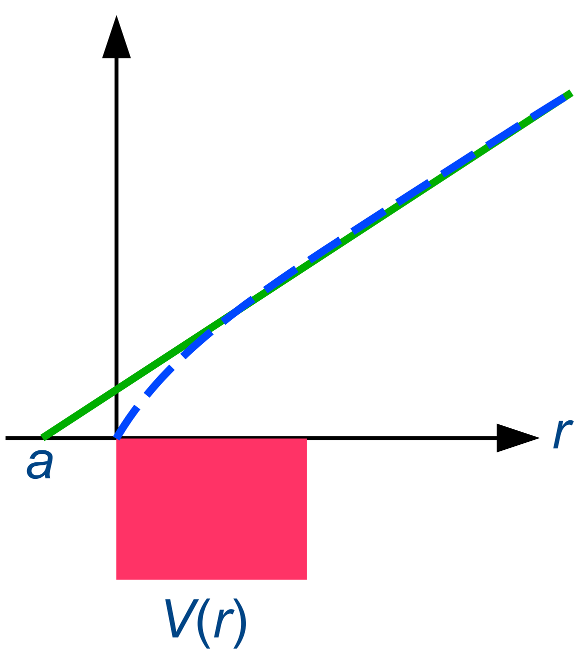
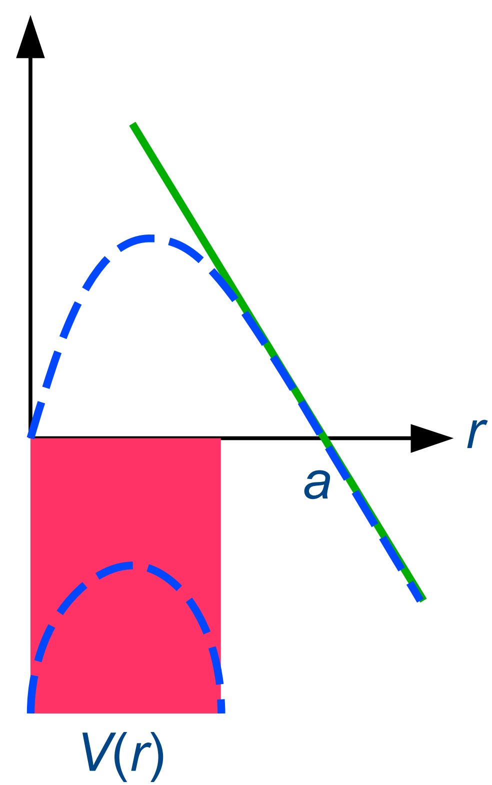


Underlying attractive

Effective repulsive



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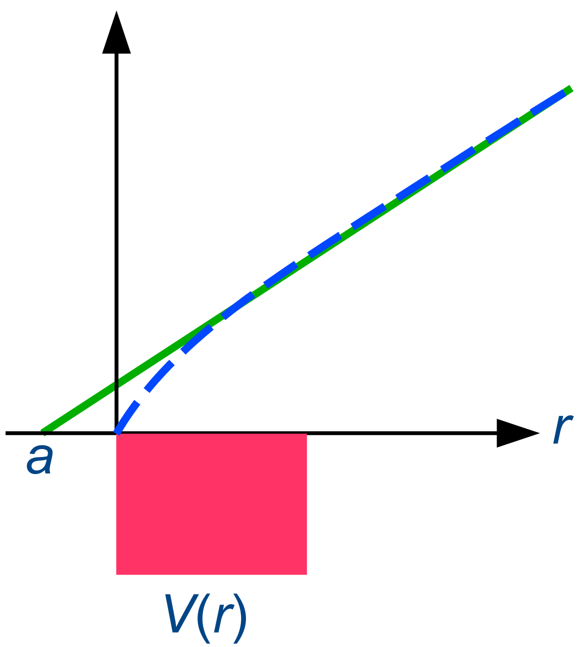
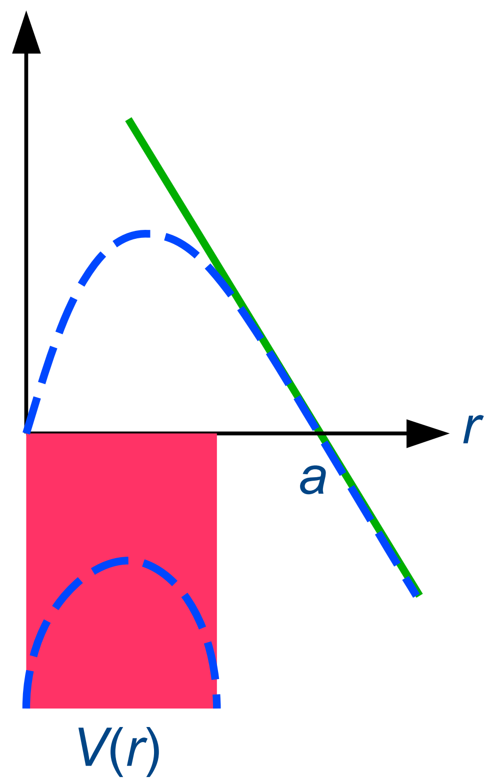


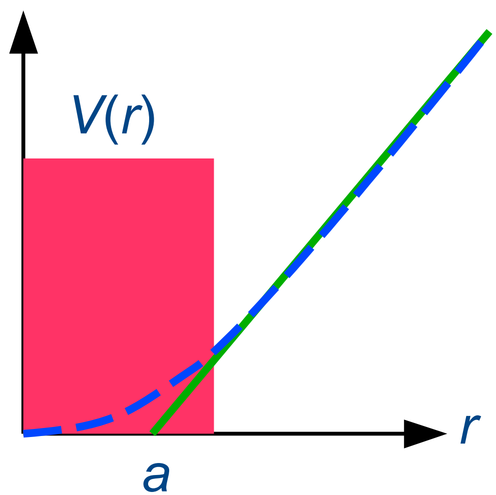
Underlying attractive

Effective repulsive

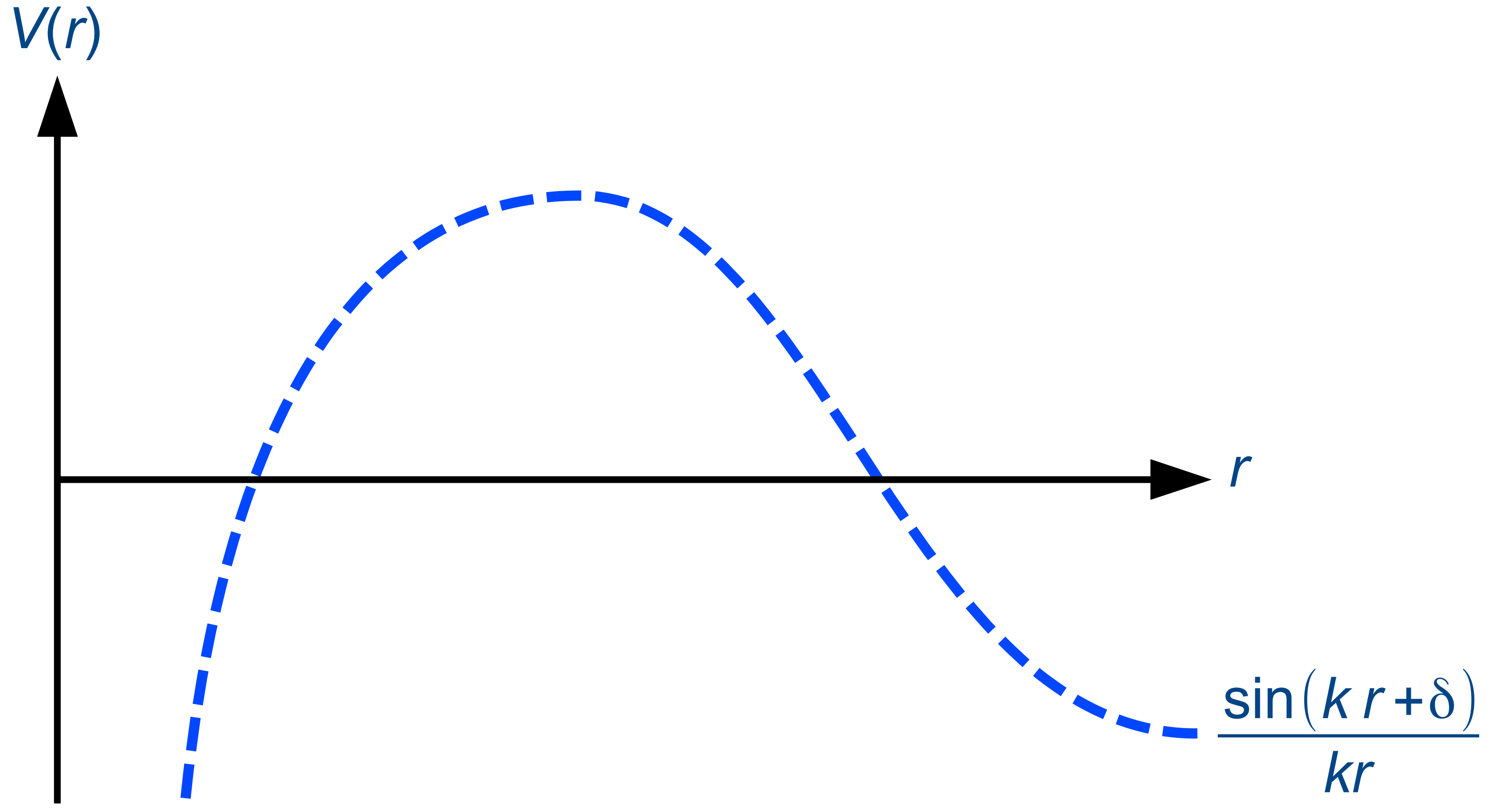


Underlying repulsive

Effective repulsive



Construction of a pseudopotential



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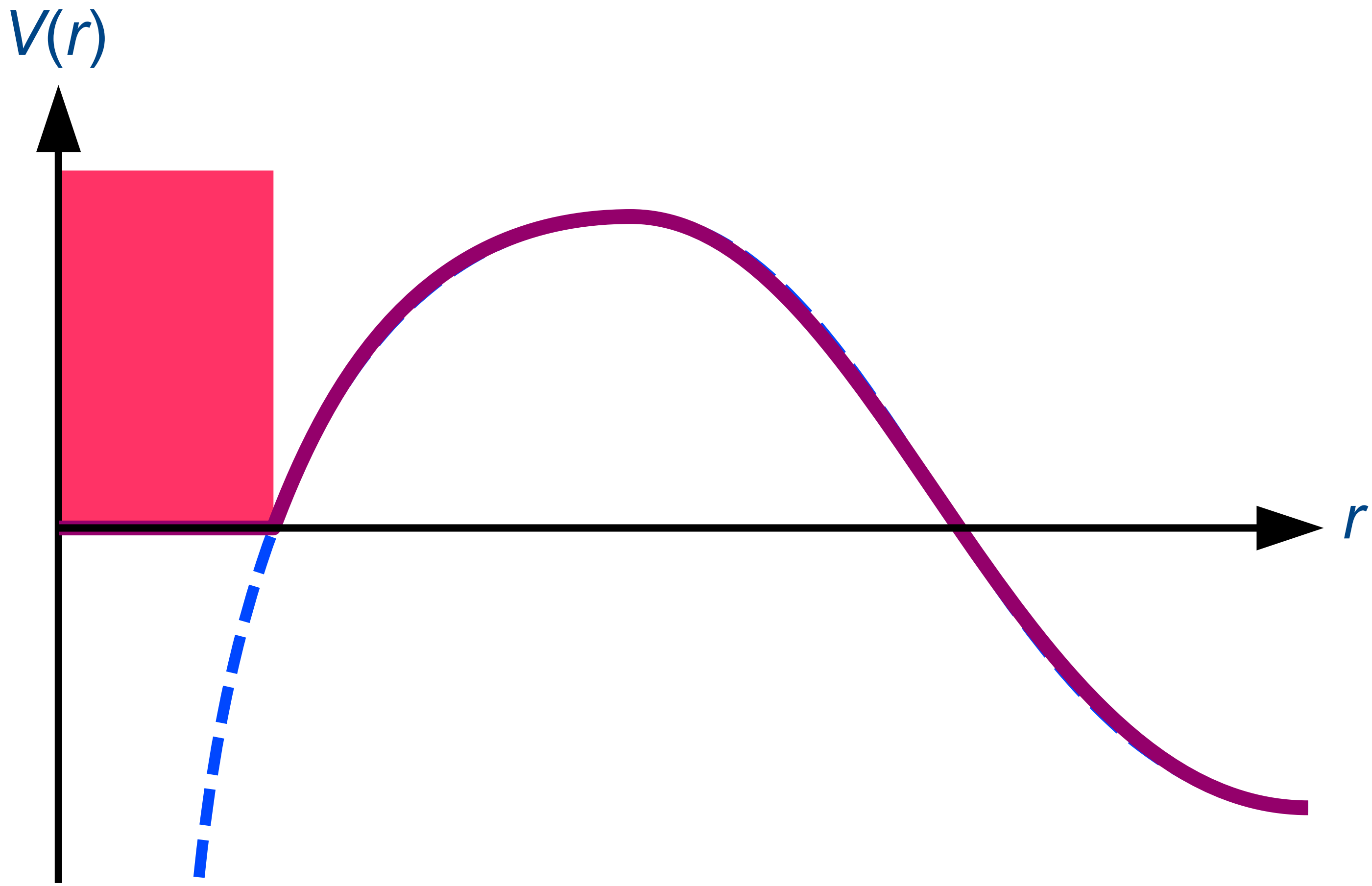

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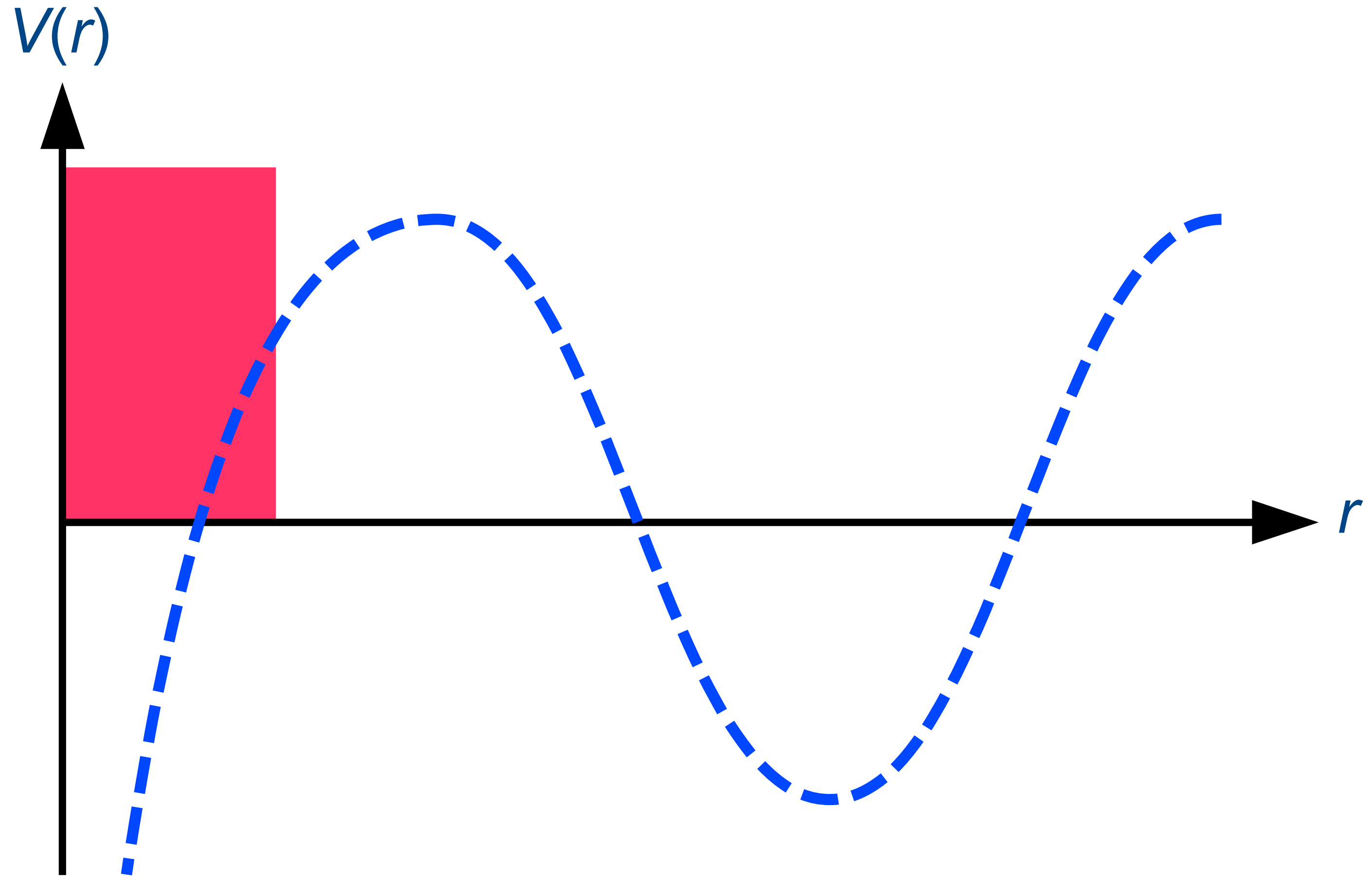

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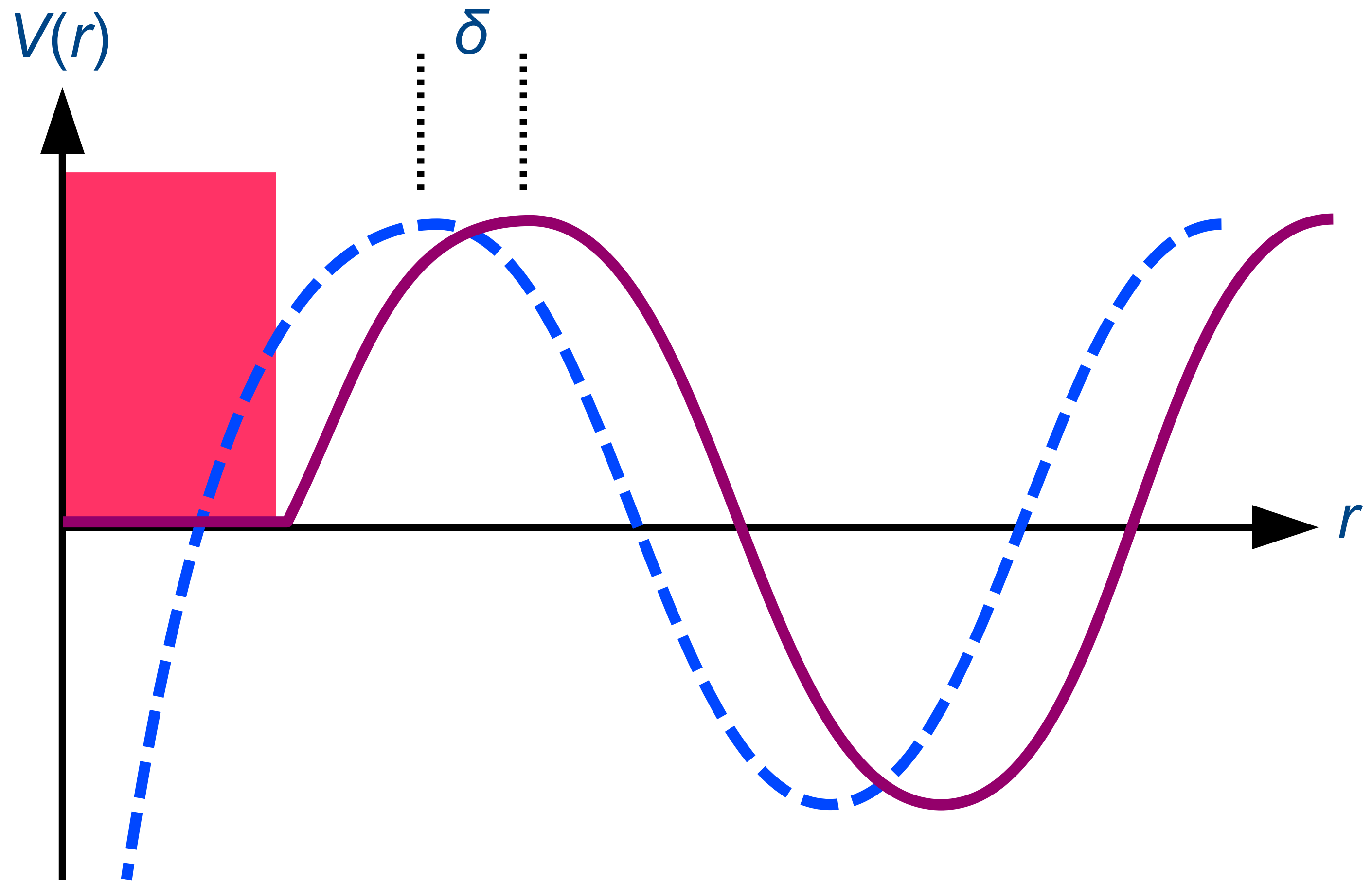

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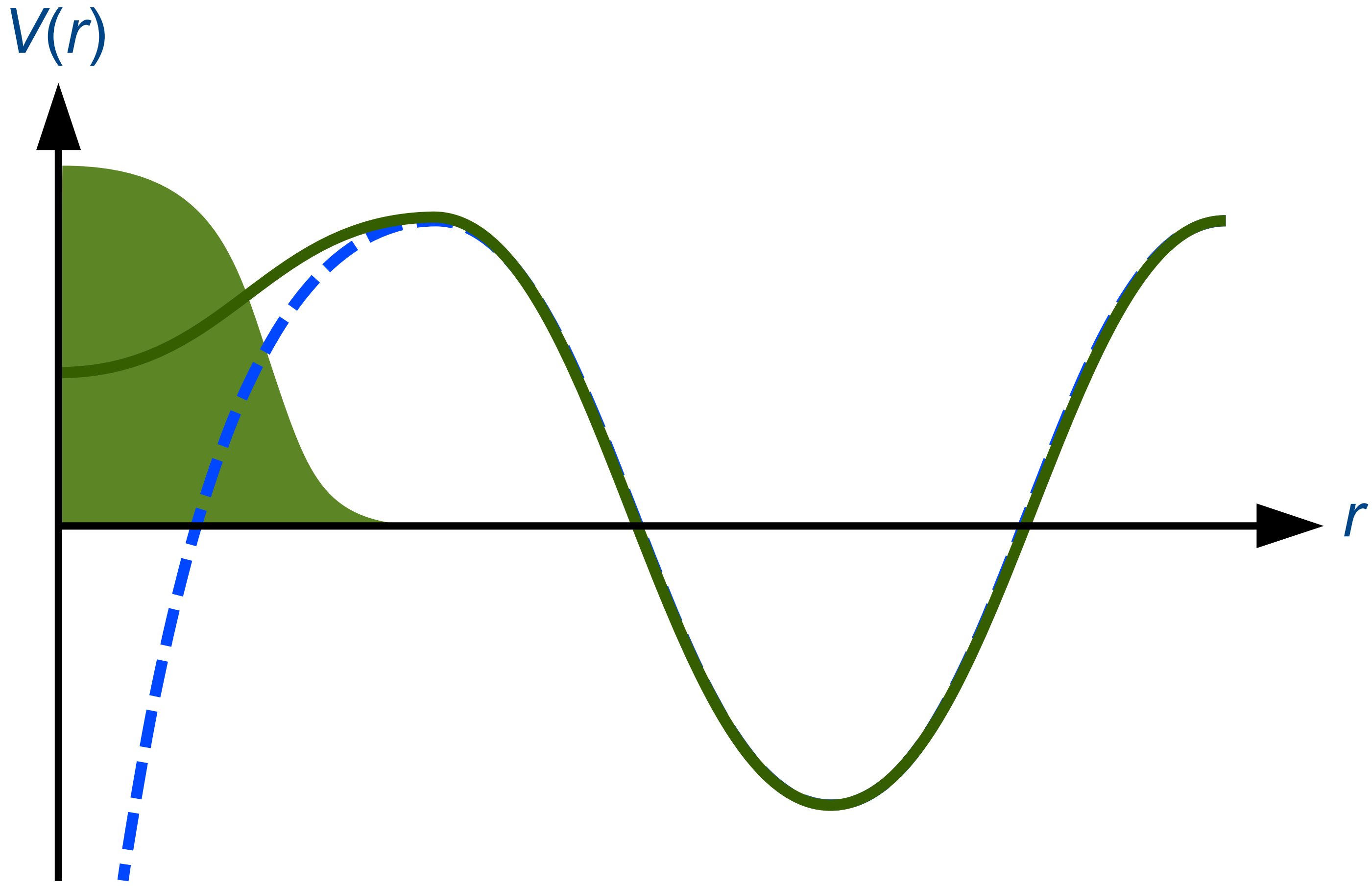
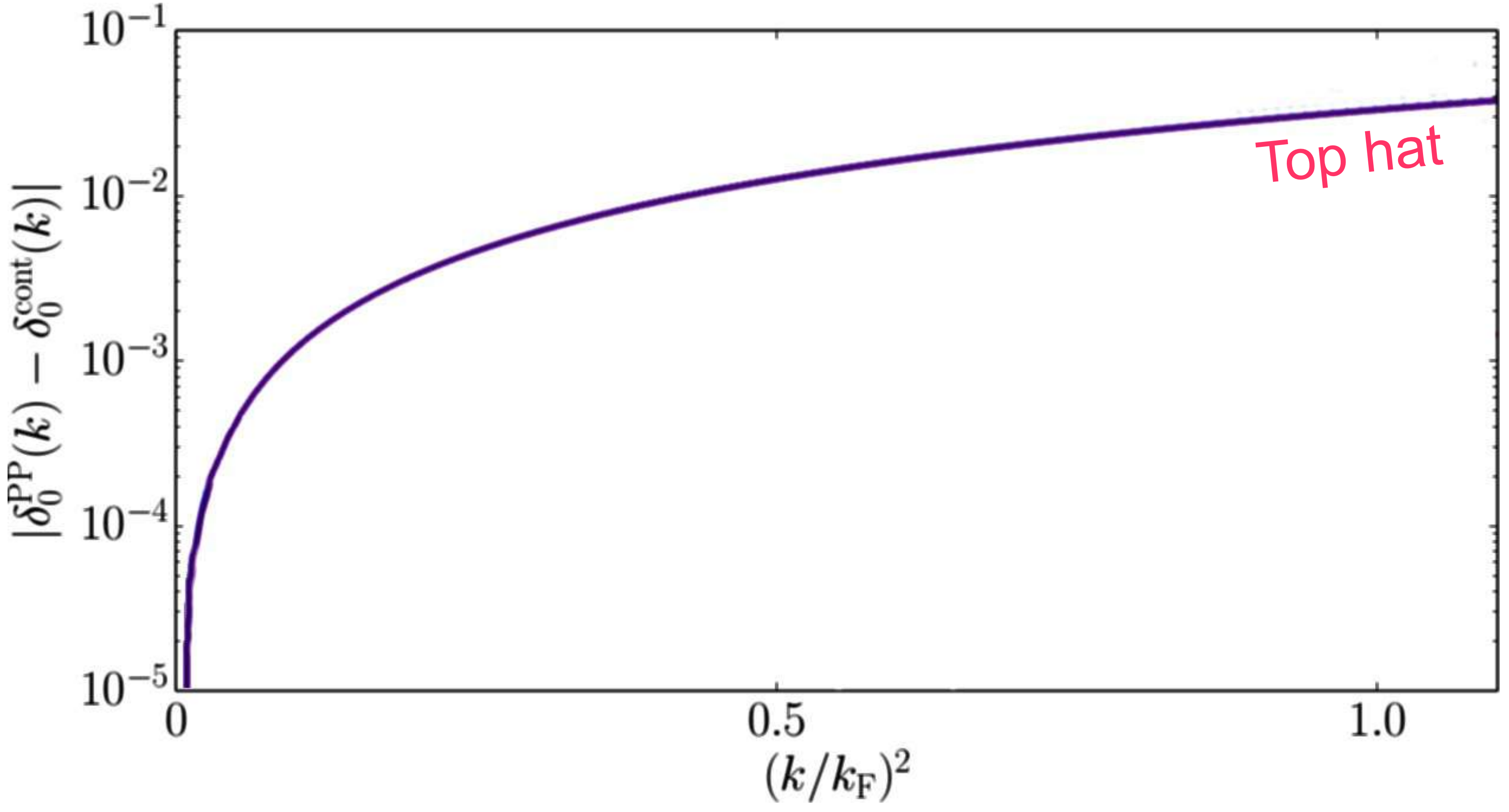
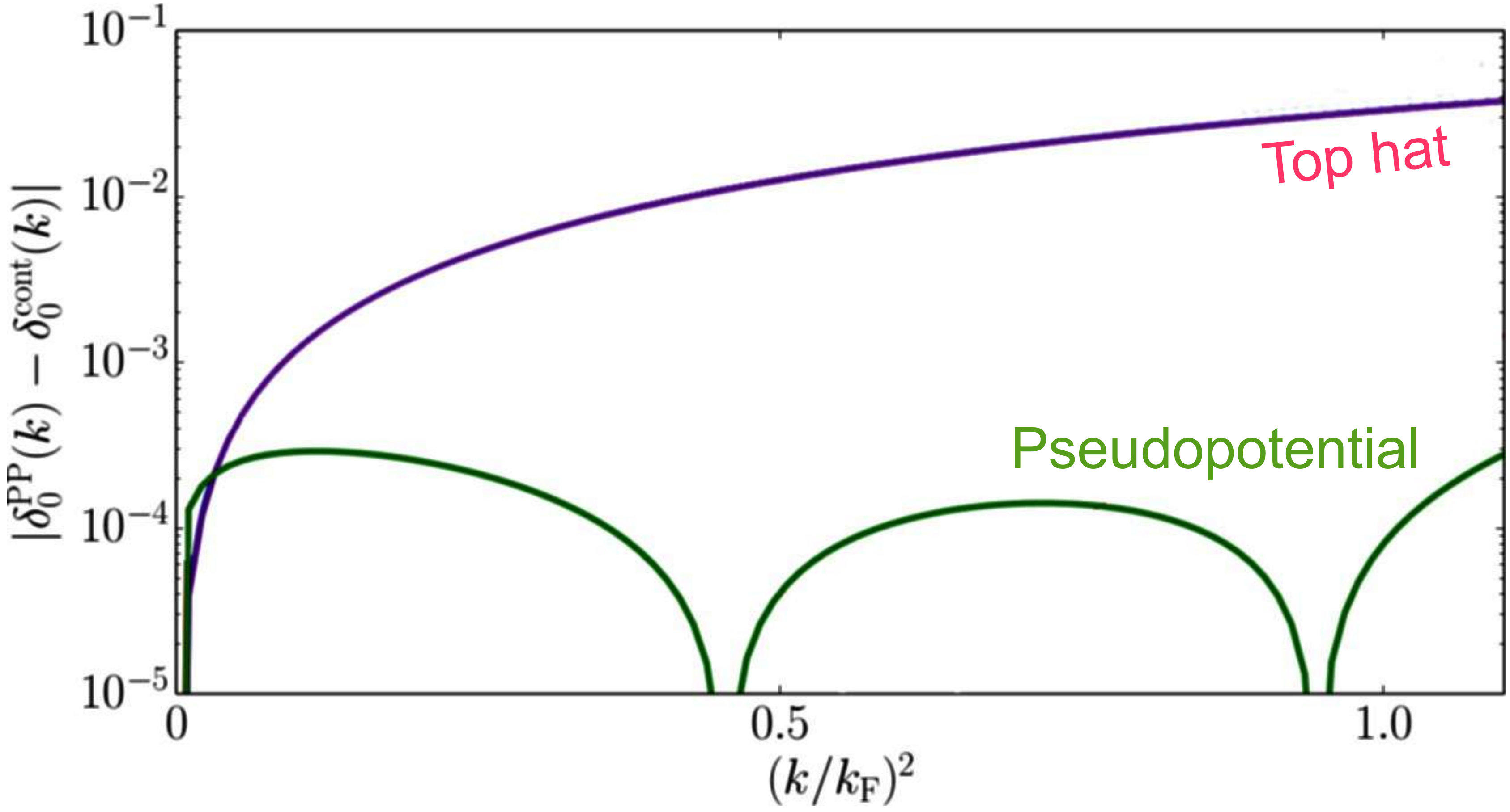


Pseudopotential: scattering properties



Pseudopotential: scattering properties



Pseudopotentials summary

Repulsive & attractive state: 100 times more accurate, 1000 times faster

Bound state: 1000 times more accurate, 1000 times faster

Stoner Hamiltonian

$$H = -\frac{\nabla^2}{2} + 4\pi a\,\delta(\boldsymbol{r}_\uparrow - \boldsymbol{r}_\downarrow)$$

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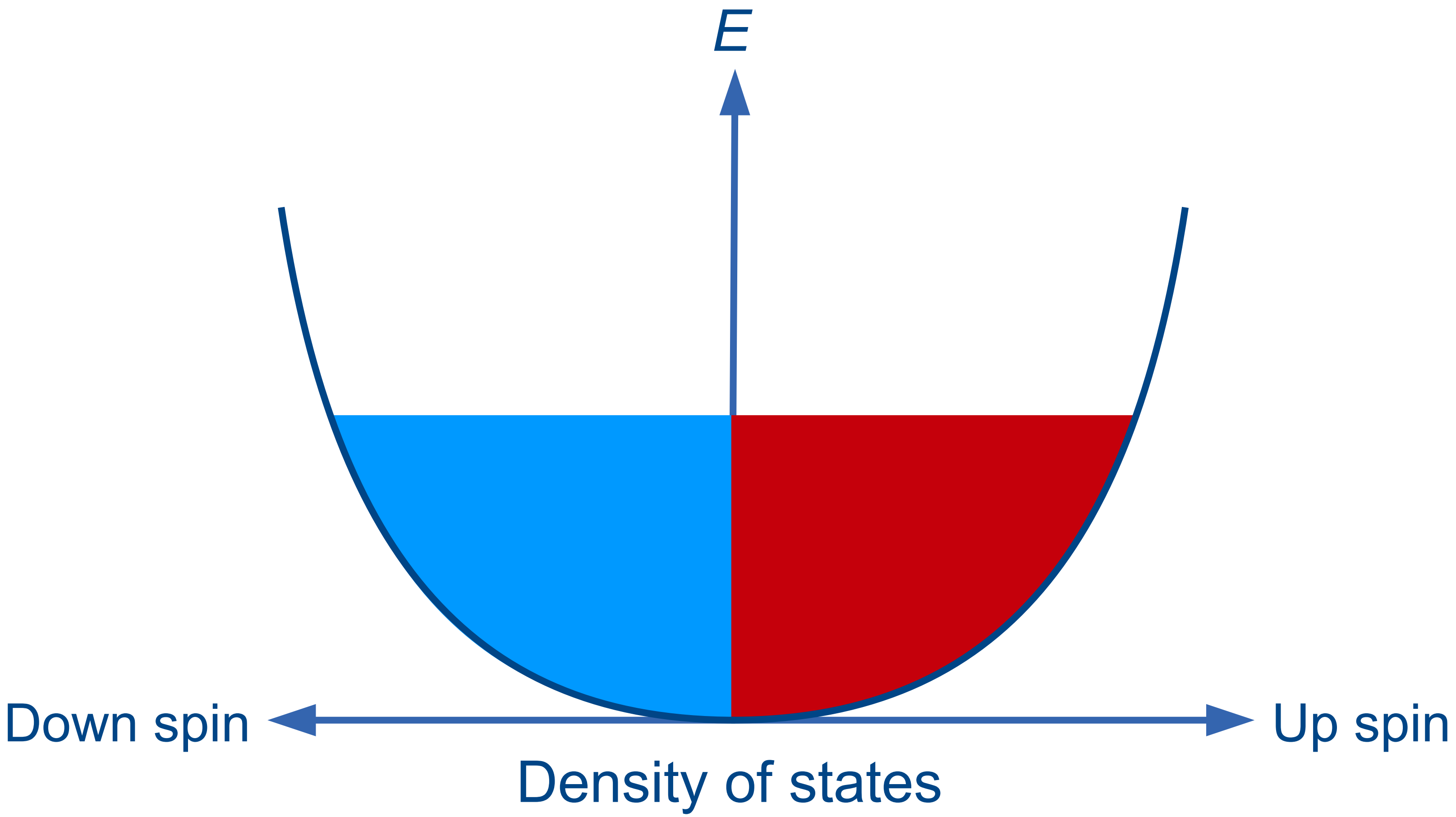

Stoner Hamiltonian

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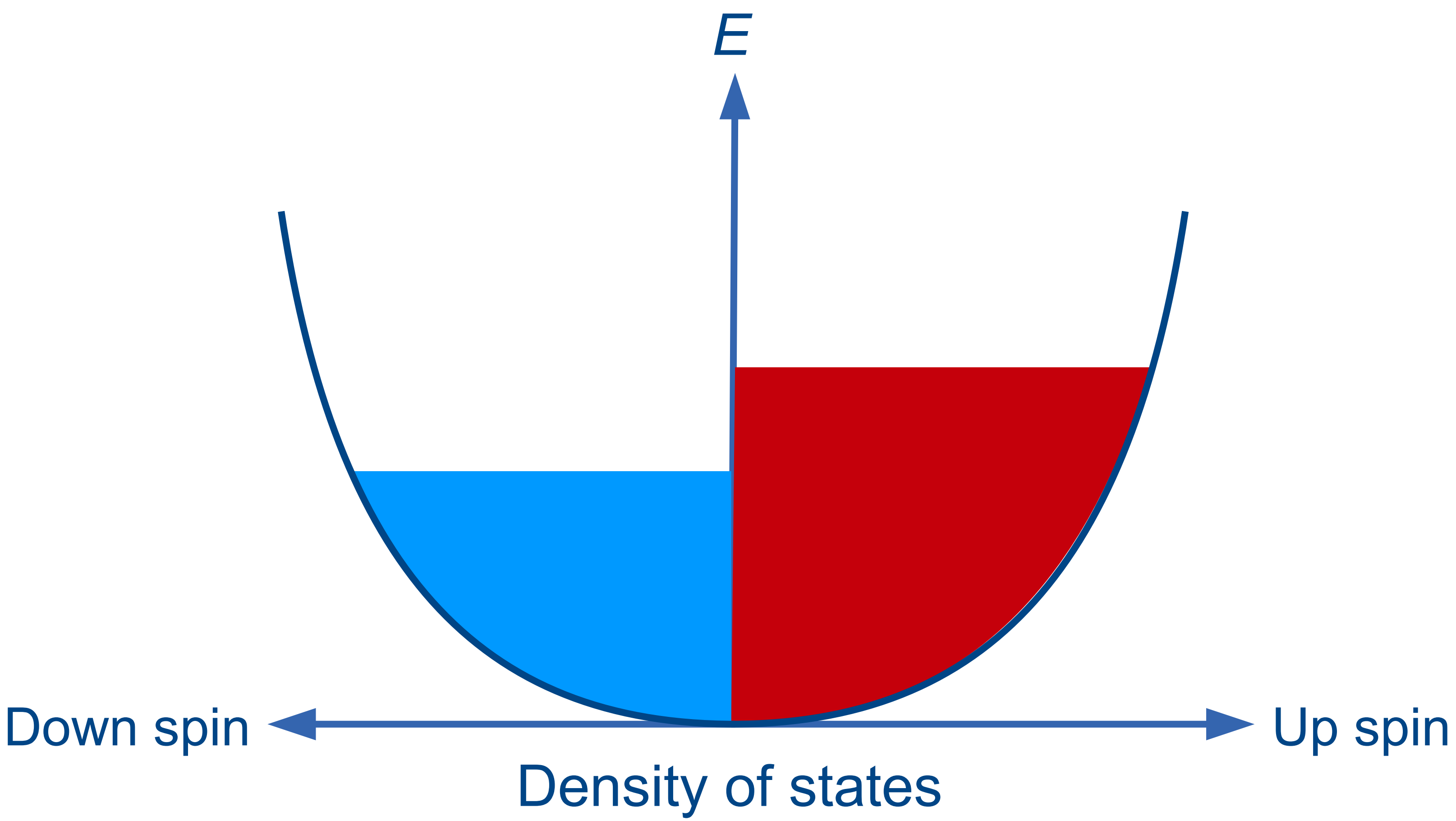
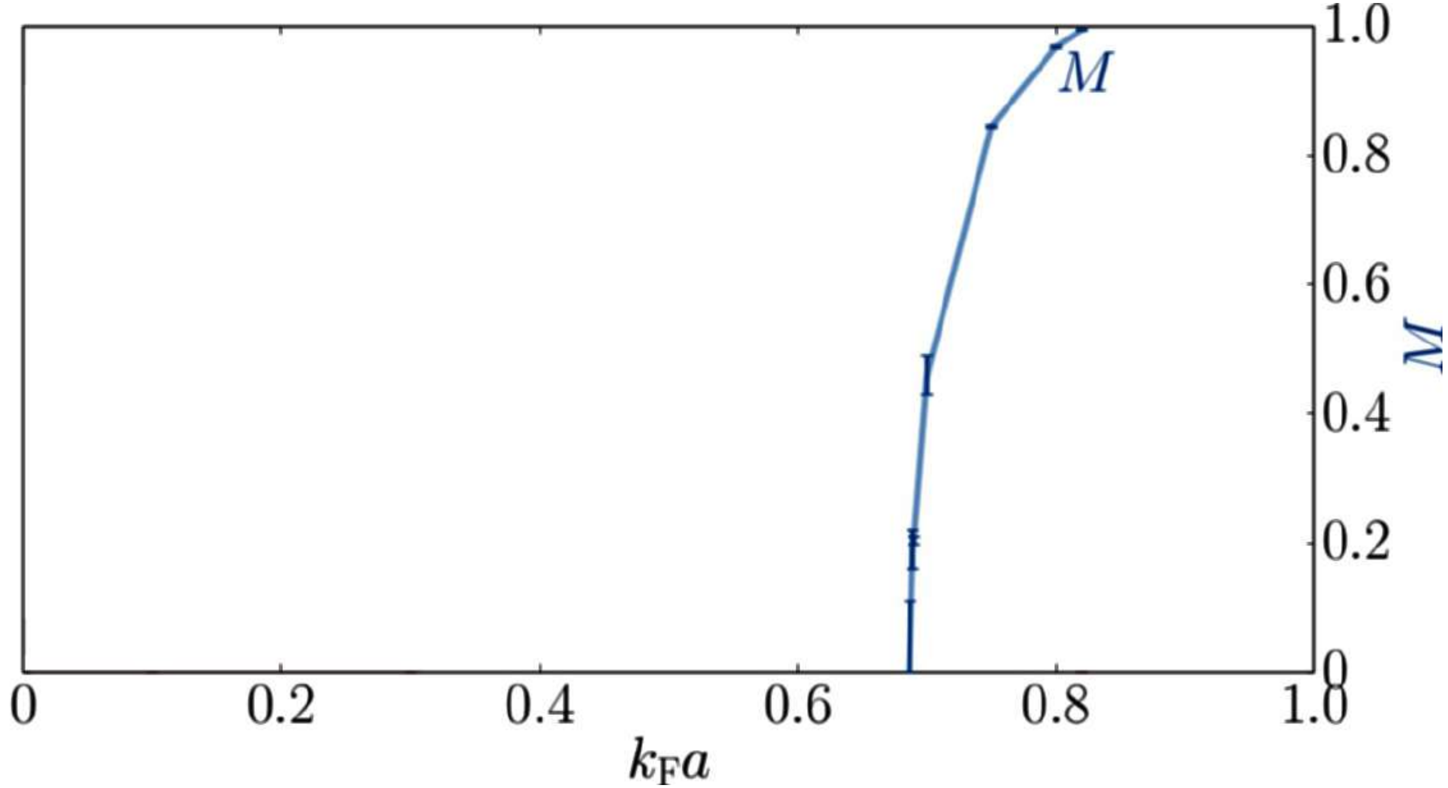


Theories of ferromagnetism

Stoner mean-field theory	Second order	$k_F a=1.57$
Fluctuations beyond Hertz-Millis	First order	-
Polaron theory	First order	-
Field theory	First order	$k_F a=1.054$
Tan relations	No magnetism	-
DMC hard sphere	First order	$k_F a=0.81(2)$
Hartree Fock MC	First / second order	$k_F a=0.83(2)$

Emergence of ferromagnetism



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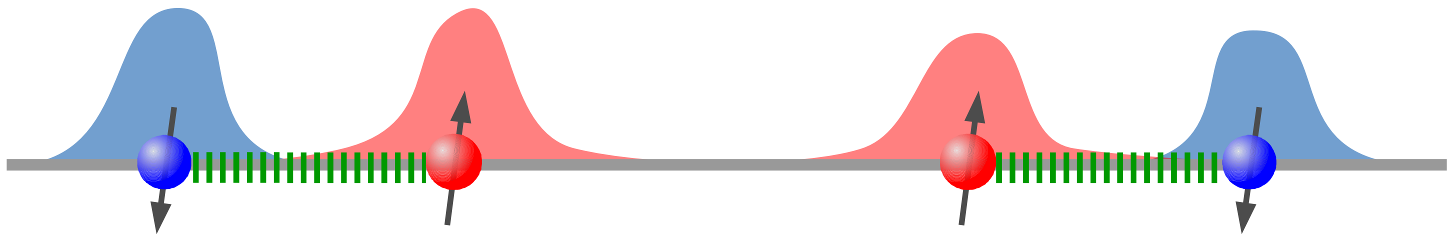
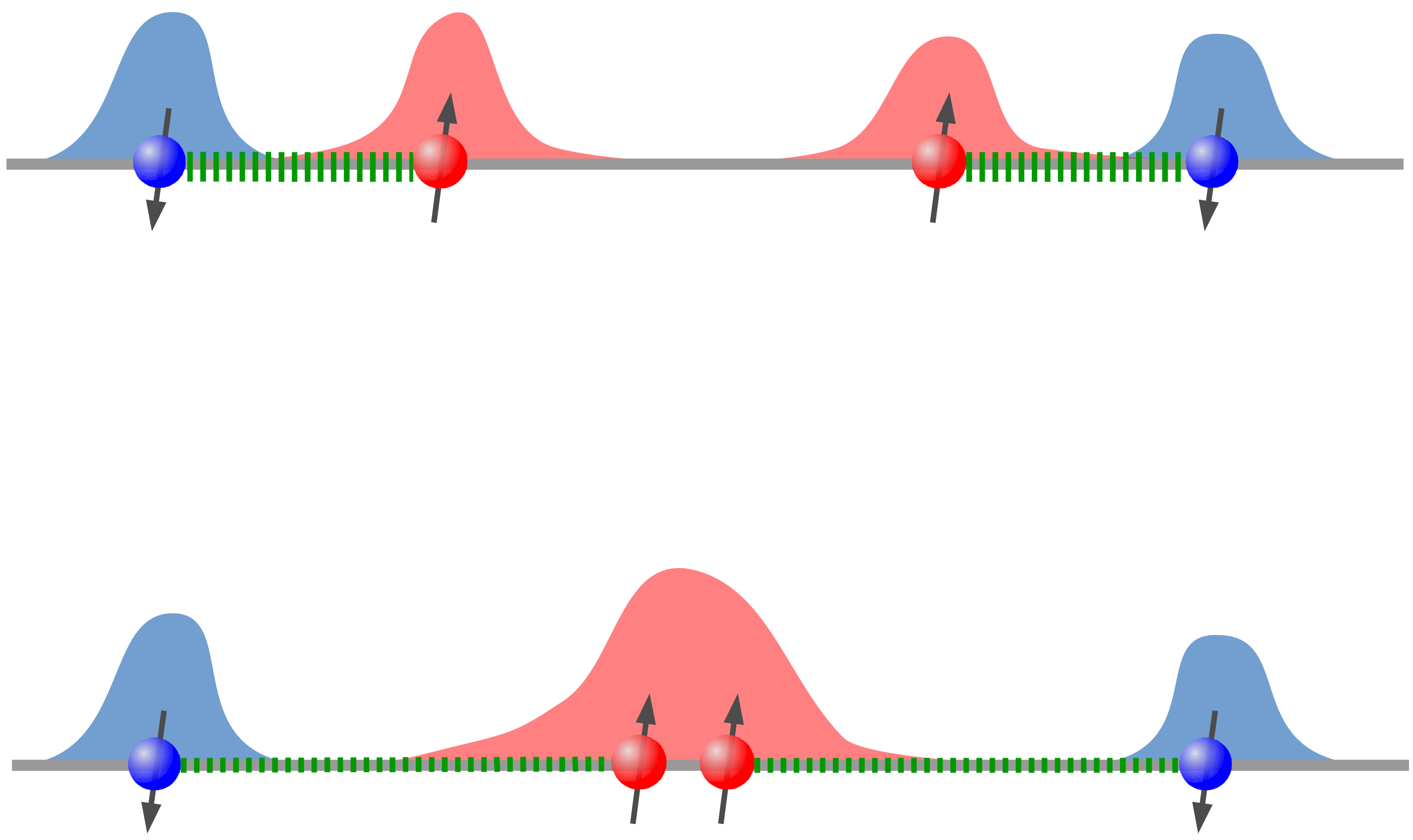
DMC hard sphere	First order	$k_F a=0.81(2)$
Hartree Fock MC	First / second order	$k_F a=0.83(2)$
DMC pseudopotential	Second order	$k_F a=0.683(1)$

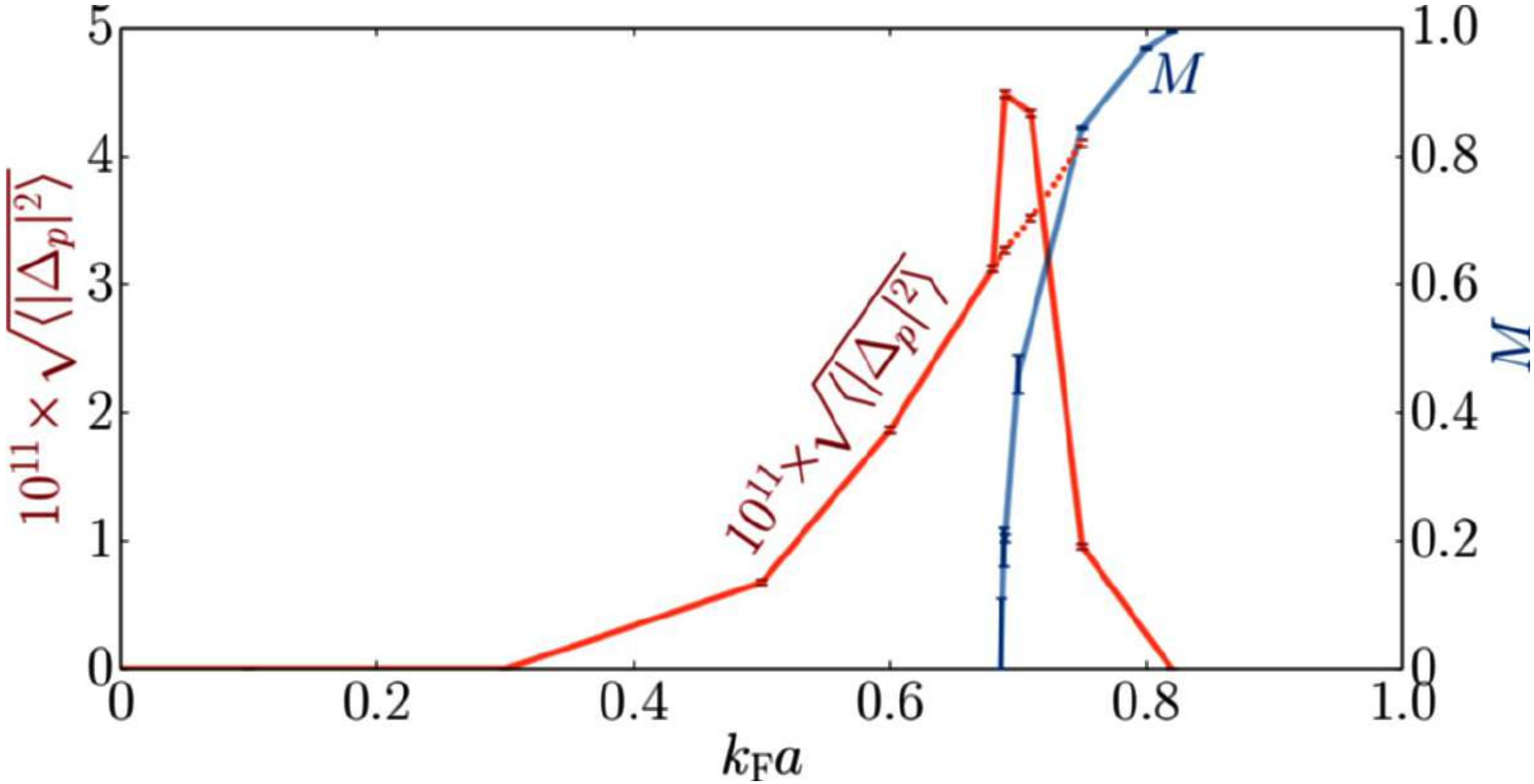
Fluctuation contributions



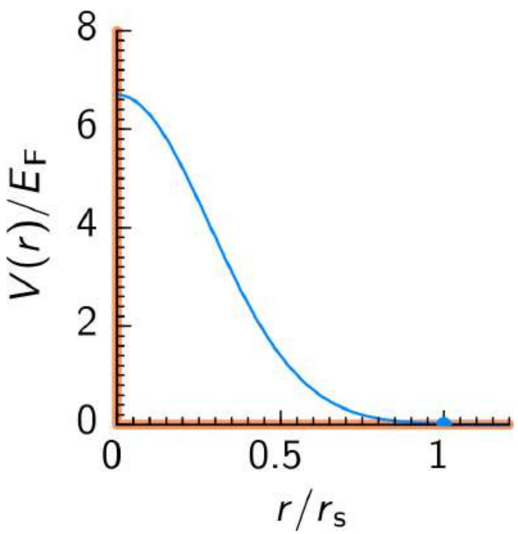
Fluctuation contributions

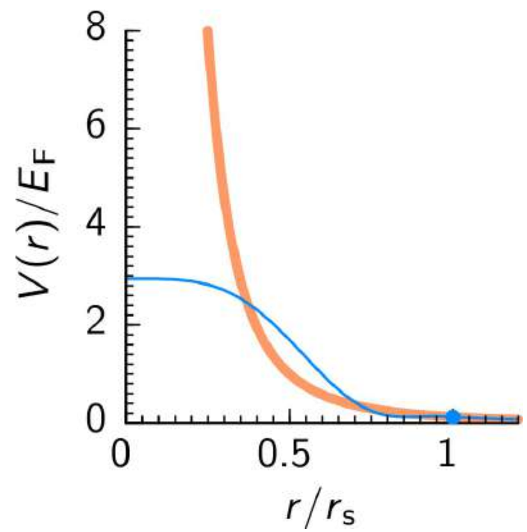


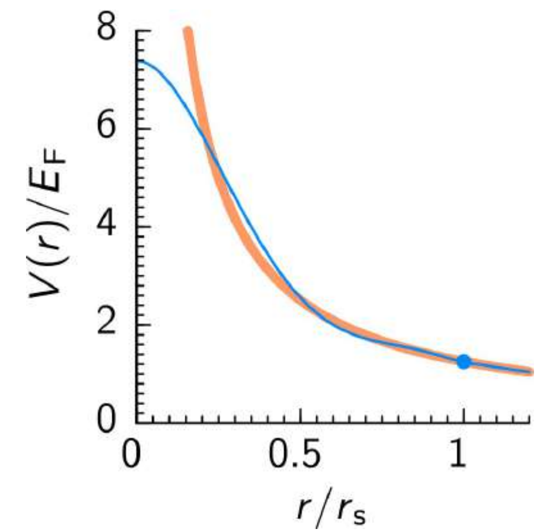
Emergence of p-wave superconductivity



Other pseudopotentials





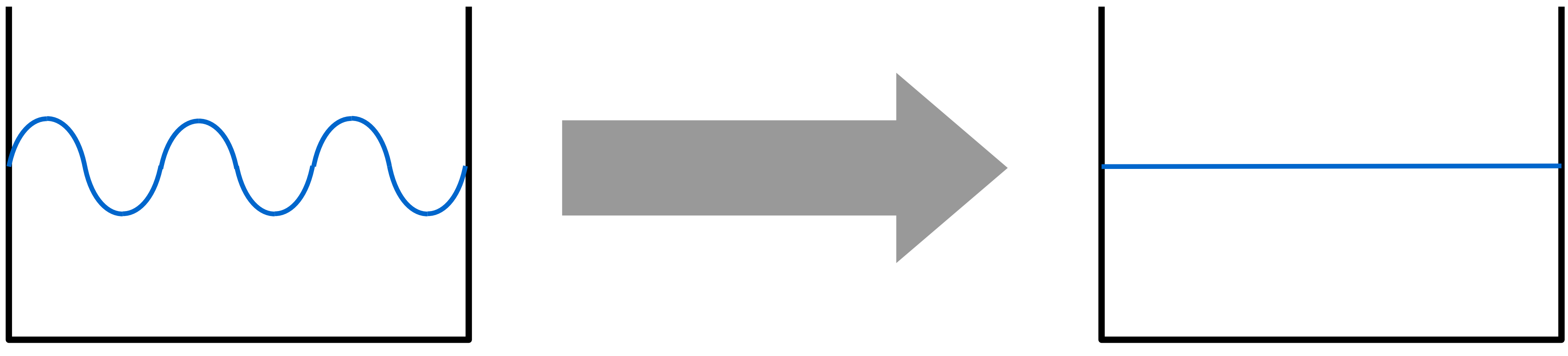


Contact	Dipolar (Whitehead)	Coulomb
1000 times faster	450 times faster	30 times faster

Kinetic energy pseudization

$$H = KE + V_{e\text{-}i} + V_{e\text{-}e}$$

Smooth integrand



Summary

Developed a pseudopotential for the contact, dipolar, and Coulomb interactions

Proposed a scheme to smooth the kinetic energy

Stoner Hamiltonian displays second order ferromagnetic phase transition and p-wave ordering

Construction of a pseudopotential

$$V_{\mathrm{PP}}(r) = \begin{cases} \dfrac{1}{c} + \left(1 - \dfrac{r}{c}\right)^2 \left[v_1 \left(\dfrac{1}{2} + \dfrac{r}{c} \right) + \sum_{i=2}^{N_v} v_i \left(\dfrac{r}{c} \right)^i \right] & r < c \\ \dfrac{1}{r} & r > c \end{cases}$$

$$\sum_{l=0}^{l_{\max}} \int_0^{k_F} \left[\left.\frac{\mathrm{d} \ln \psi_{\mathrm{PP}}(k,l)}{\mathrm{d} r}\right|_c - \left.\frac{\mathrm{d} \ln \psi_{\mathrm{cont}}(k,l)}{\mathrm{d} r}\right|_c \right]^2 \mathrm{d}k$$